

Cover page

## Seeing atoms only 0.78Å apart

M.A. O'Keefe and E.C. Nelson

National Center for Electron Microscopy, LBNL B72, Berkeley, CA 94720, USA

### DISCLAIMER

-----  
*This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor The Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or The Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, or The Regents of the University of California.*

*Ernest Orlando Lawrence Berkeley National Laboratory is an equal opportunity employer.*

-----  
*Ernest Orlando Lawrence Berkeley National Laboratory -- LBNL-52325*

## Seeing atoms only 0.78Å apart

M.A. O’Keefe and E.C. Nelson

*National Center for Electron Microscopy, LBNL B72, Berkeley, CA 94720, USA*

**The one-Ångstrom microscope (OÅM) project<sup>1</sup> at the USDOE’s National Center for Electron Microscopy has extended the limits of high-resolution transmission electron microscopy to sub-Ångstrom levels. The OÅM combines image-processing software<sup>2,3</sup> with a modified 300keV electron microscope equipped with a highly-coherent field-emission electron gun<sup>4</sup>. We have found that a reduction in the OÅM’s electron-gun extraction voltage allows us to “see” silicon atoms separated by only 0.78Å.**

Transmission electron microscopy is used as an aid to the determination of microstructure. The goal of high-resolution transmission electron microscopy is imaging at the level of single atomic columns. In simple materials, such as metals viewed in easy projection directions, this goal is met at microscope resolutions of 1.5-2.0Å. Resolution requirements become more stringent in more complex projection directions – only 1.9Å resolution is needed to separate silicon atoms in [001] orientation, compared with 1.36Å in [110] and 0.78Å in [112] orientations. Better microscope resolutions allow us to see the atoms in materials in many more projection directions – an important consideration for determination of three-dimensional microstructure.

Smaller atoms are more tightly packed and require higher resolution. In [110] orientation, a resolution of 1.36Å is sufficient to separate silicon atom columns, but diamond requires 0.89Å resolution to separate the carbon atom columns<sup>5</sup>. In [112] orientation, a resolution of 0.93Å separates the Cd and Te columns in CdTe<sup>6</sup>, but a resolution of 0.78Å is needed for silicon. In

addition, defects such as dislocation cores, in which atoms are not arranged periodically, require sub-Ångstrom resolution<sup>7</sup>, as do grain boundaries and other interfaces.

Sub-Ångstrom microscopy with a transmission electron microscope requires careful attention to detail. Lens aberrations must be minimized, power supplies must be stabilized, and the microscope environment must be optimized to reduce vibration, and acoustic and electromagnetic noise. For imaging of 0.78Å spacings at 300keV, theory requires a microscope with focus-spread of less than 20Å, three-fold astigmatism less than 460Å, specimen vibration less than 0.35Å, and a specimen less than 65Å thick<sup>4</sup>. We achieved sub-Ångstrom resolution with the OÅM installed in a specially-designed room<sup>8</sup>, and its residual three-fold astigmatism reduced to 300Å with a hardware corrector. Its spread of focus was minimized to 20Å for a theoretical “information limit” of 0.8Å. Initial tests with a diamond specimen showed that the corrected OÅM could successfully resolve the 0.89Å (004) atom pairs in [110] diamond.<sup>4,5,9</sup>

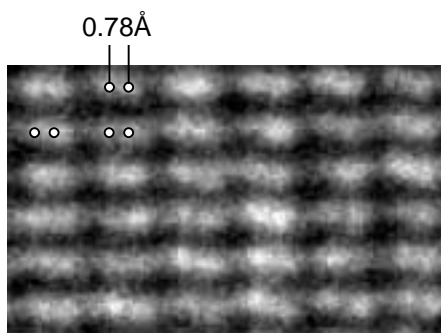
Reducing the electron-gun extraction voltage from a normal 4kV lowers the microscope focus-spread, and improves its information limit, at the cost of reduced illumination. As a test, we have used a 3kV extraction voltage (for a theoretical information limit of 0.72Å) to image 0.78Å (444) atom pairs in [112] silicon. At this extreme limit of the microscope’s performance, the signal from the necessarily-thin specimen is weak and images are noisy. However, we have seen 0.78Å atom pairs at both “black-atoms” and “white-atoms” defocus (Fig. 1), indicating linear transfer of 0.78Å spacings from the specimen to the image.

Our image is a harbinger of those to be expected from the coming generation of computer-controlled, aberration-corrected, transmission electron microscopes with available sub-Ångstrom resolution.

## References:

---

1. O'Keefe, M.A. *Microstructure of Materials*, ed. K. Krishnan 121-126 (1993).
2. Coene, W.M.J., Thust, A., Op de Beeck, M. and Van Dyck, D., *Ultramicroscopy* **64** 109-135 (1996).
3. Thust, A., Coene, W.M.J., Op de Beeck, M. and Van Dyck, D., *Ultramicroscopy* **64** 211-230 (1996).
4. O'Keefe et al. *Ultramicroscopy* **89**, 4: 215-241 (2001).
5. Wang, Y.C. et al. in *57th Ann. Proc. MSA*, Portland, Oregon 822-823 (1999).
6. Nellist, P.D. and Pennycook, S.J., *Phys. Rev. Letts.* **81**, 4156-4159 (1998).
7. Kisielowski, C. et al. in *58th Ann. Proc. MSA*, Philadelphia, Pennsylvania 16-17 (2000).
8. Turner, J.H., O'Keefe, M.A. and Mueller, R. in *55th Ann. Proc. MSA*, Cleveland, Ohio 1177-1178 (1997).
9. O'Keefe, M.A. in *58th Ann. Proc. MSA*, Philadelphia, Pennsylvania 1192-1193 (2000).



**Figure 1** “White atoms” image of silicon in [112] orientation shows atom pairs at a resolution of 0.78Å and a magnification of 30 million times. Positions of three of the atom pairs are marked by white dots.